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6. AUTHOR(S)
Cathleen Morawetz

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
New York University Courant Institute of Mathematical Sciences
251 Mercer Street
New York, NY 10012

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New York University
Courant Institute of Mathematical Sciences
251 Mercer Street
New York, N.Y. 10012

# FINAL REPORT

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Title: New Algorithms for Determining and Optimizing the Properties of Materials and Fluid Flows

Period: June 1, 1987 - October 31, 1990

Principal Investigator: Cathleen S. Morawetz



Prepared December 1990

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# Final Report
# DARPA Grant F49620-87-C-0065
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## General Survey

The principle goal of the work done on DARPA Grant No. F49620-87-C-0065 has been to produce new algorithms for solving problems in the properties of fluids and solids and to find new techniques for the parallelization of algorithms. Foci have been on algorithms for the non-destructive testing of objects, the optimization of structures, the computational analysis of phase change, the parallelization of linear algebra and other basic algorithms. Other topics have been involved because of their intimate connection either to parellelizaton (e.g. queueing theory), to materials, or to numerical methods for relevant p.d.e.'s including nonlinear hyperbolic methods themselves.

This report consists of a summary of the topics studied, the investigators and short outlines of their achievements. These are grouped under the titles. Algorithms for Materials, Parallelization of Algorithms, Other topics. A general description is followed by longer reports covering the past year and a half of activity, a bibliography of work published and a list of researchers and students supported.

## Algorithms for Materials

This work was conducted mainly under the guidance of R. Kohn, J. Goodman and C.S. Morawetz. It involved as well G. Allaire, S. Cox, A. Szepassy, J. Sylvester, John Strain, M. Landman and Paula Whitlock. The areas were structural optimization, electrical impedance tomography.

### Structural Optimization

The goal of structural optimization is to choose the geometry or composition of a load-bearing structure so as to optimize its performance for a given amount of material.

S. Cox worked with M. Overton on non-smooth optimization problems arising in the optimal design of columns against buckling. Prior work had been based primarily on necessary

conditions, and contained mistakes that had led to much controversy in the literature. Cox and Overton corrected those mistakes, and showed that the problem can actually be solved by a direct optimization scheme. The associated mathematical programming problem is non-smooth, because the buckling load of an optimal column is usually a multiple eigenvalue of the associated differential equation. This work was reported in "On the optimal design of columns against buckling," by S. Cox and M. Overton, to appear in *SIAM Journal of Mathematical Analysis*.

R. Kohn and G. Allaire explored the shape optimization of two-dimensional structures in plane stress. They implemented a new approach, based on the introduction of "composite materials" as design elements. This amounts to permitting subgrid structure, hence to enlarging the apparent design space. The result is an approach to structural optimization that is more global in character - with fewer local minima than conventional methods. This work is now being prepared for publication in the form of an article "Optimal design for plane stress using composite materials," by G. Allaire and R. Kohn.

R. Kohn also explored a connection between optimal design and coherent phase transitions. The latter is actually also a problem of optimal design - in which the quantity to be optimized is a thermodynamic free energy. The "composite materials" discussed above correspond to the microstructures of phase mixtures created by coherent phase transitions. Kohn explored the metallurgical literature in this area, which goes back to the 1960's, and explained its relation to the recent work on structural optimizaton. This work is reported in the "The relaxation of a double-well energy," by R. Kohn, to appear in *Continuum Mechanics & Thermodynamics*.

**Electrical Impedance Tomography**

The goal of electrical impedance tomography is to image the interior conductivity of an object by menas of low-frequency voltage and current-flux measurements at the boundary. This is a promising new approach to nondestructive testing. It has also been proposed for a variety of biophysical and geophysical applications.

R. Kohn and A. McKenney explored the implementation of a new variational approach to this inverse problem. They developed a Newton-type minimization scheme, and explored the performance of the method in a two-dimensional setting. It was found to be surprisingly stable in

the presence of noise, provided that the boundary currents are not too localized. This work was reported in "Numerical implementation of a variational method for electrical impedance tomography," by R. Kohn and A. McKenney, *Inverse Problems* b, 1990, 389-414.

J. Sylvester explored the imaging of locally anisotrophic conductivities. Here there is a problem of non-uniqueness: different bodies can give the same boundary measurements if they are related - "by change of variables." Sylvester proved the converse, in two dimensions: two bodies that are indistinguishable by boundary measurements must be related in this way. His work is reported in "An anisotropic inverse boundary value problem," by J. Sylvester, *Comm. Pure Appl. Math.* 43, 1990, 201-232.

**Other Inverse Problems**

C.S. Morawetz studied two numerical problems in inverse scattering in two space and one time dimensions for the wave equation. The basic solutions are: in free space a plane wave for problem I and a fundamental solution for problem II. Problem I is the classical problem of determining a potential from data at infinity scattered back in the direction from which the wave came. All directions of the initial wave then give enough data. Problem II is to determine a smooth sound speed form data collected on a fixed line for all time. This problem is ill-posed and one can only ask what if anything can be determined about the sound speed.

The corresponding direct problems are analyzed through computed examples. In Problem I some very interesting properties, discovered by Ralston and Eskin, of the scattered field interfere with the computation of the inverse and it is impossible to make a very logical looking algorithm converge. In Problem II for the direct problem a back scattered field was obtained showing a wave running across the line. The first part of this work was reported in "Scattering by a Potential Using Hyperbolic Methods", by A. Bayliss, Y. Li and C.S. Morawetz, *Mathematics of Computation*, Vol. 52, Number 186, pp. 321-388, (1989). The second part in "On 2D Inverse Scattering", to appear in *The Proceedings of the International Conference on the Mathematical and Numerical Aspects of Wave Propagation*, to be published in March 1991 by SIAM.

**Crystal Growth**

Crystal growth computations were made by John Strain with James Sethian (UC Berkeley). They wrote and debugged a code for solving a Stefan problem with curvature-dependent boundary conditions. The code uses a level set formulation of the moving boundary problem, with heat potential theory to reduce the heat equation to the moving boundary. A fast algorithm is used to evaluate the heat potential, yielding an optimal algorithm which is capable of treating completely arbitrary geometries. This research is described in the forthcoming paper "Crystal growth and Unstable Solidification".

Strain also developed a new family of fast algorithms for classical potential theory, based on Ewald summation. These algorithms evaluate classical layer or volume potentials, or discrete sums, formed with the Green function for a cube. This research is described in "Fast Potential Theory I: Poisson Solvers on a Cube," Center for Pure and Applied mathematics (UC Berkeley) Report PAM-480, December 1989, and submitted to Math. Comp. and "Fast Potential II: Layers Potentials and Discrete Sums," Center for Pure and Applied Mathematics (UC Berkeley) Report PAM, April 1990, submitted to *Jour. Comput. Phys.*

Further work has been on quasistationary crystal growth problems using integral equations, level sets and the fast algorithms described above as well as the construction of a fast Laplace transform based on Laguerre functions; it is described in "A Fast Laplace Transform Based on Laguerre Functions," submitted to *Math. Comp.*

With Leslie Greengard, he constructed a fast algorithm for evaluating Gaussian convolution sums, "The Fast Gauss Transform," to appear in *SIAM J. Sci. Stat. Comput.* This work was extended to evaluate Gaussian convolution sums with variances which vary from point to point, "A Fast Gauss Transform with Variable Variances," submitted to *SIAM J. Sci. Stat. Comput.*

**Fast Monte-Carlo Methods:**

J. Goodman, with A. Sokal, completed a study with theory and numerical experiments on their multiscale algorithm, Multigrid Monte-Carlo, for rapid simulation of random fields.They also generalized the method to other models, such as the XY model, with significant success. These are reported in, "Multi-Grid Monte Carlo I. Conceptual Foundations", J. Goodman and A.

D. Sokal, *Phys. Rev A. (1989)* and "Multi-Grid Monte Carlo II. Two-Dimensional XY Model", R. Edwards , J. Goodman and A. Sokal, to appear in *Nuclear Physics B.*

**Monte Carlo Methods in Phase Transition**

Paula A. Whitlock has focussed on the simulation of quantum systems using Monte Carlo methods. The distinct areas have been 1) the simulation of helium films physisorbed on a substrate; 2) first principles calculation of two and three body interactions and 3) development of Green's function Monte Carlo method employing the recently developed "shadow" trial wave function for quantum many-body systems. All these areas share a common use of development of quantum Monte Carlo methods.

The ground-state properties of liquid and solid helium are, to a large extent, well understood. However, helium systems with interfaces, while extensively studied experimentally, are just beginning to be understood by theoreticians. Whitlock is systematically studying helium adsorbed on graphite using Monte Carlo methods. Helium films are particularly simple and their basic properties such as film growth, the characteristics of the films two-dimensional phases, and their melting-freezing transitions can be investigated theoretically and compared wtih these phenomena theoretically at the microscopic level, as well as calculating from microscopic theory the parameters that go into empirically-derived theories.

The approach to the study of helium films is to perform variational Monte Carlo and Green's function Monte Carlo (GFMC) simulations. The GFMC method was first introduced by Kalos and was further refined by Kalos, Levesque and Verlet The form of GFMC used corresponds to resolvent methods in many-body perturbation theory. The relevant equation is iterated many times, it converges exponentially and exactly to the lowest state of the Hamiltonian which is not orthogonal to the starting wave function. The iterations are carried out by random walks starting with an optimized trail wave function. No other method is available for many-body systems which can evaluate the ground state and orthogonal excited states of the Schrodinger equation exactly within the statistical sampling errors. The results of the calculation are sets of particle configurations whose probability density represent the ground state of the system. These particle configuration are used to form expectation values to compute observables of the

system.

A variety of phenomena associated with helium films have been studied. The equation of state can be computed and an investigation of the solid phases of the helium monolayer commensurate and incommensurate with the underlying graphite lattice is possible.

Whitlock also worked on determining the properties of two and three body systems through solving the Schrodinger equation exactly using Green's function Monte Carlo. Whitlock's approach to the problem, which emphasizes the role of certain interaction energies naturally divides into three parts. The first is the development of optimized wave functions to use as trial wave functions in our Monte Carlo simulations. The second part is to perform variational Monte Carlo calculations with the proposed wavefunctions and the last part is to perfom the Green's function Monte Carlo simulations. So far, efforts have been on obtaining the two and three body potentials for polarized hydrogen and helium.

## Parallelization of algorithms

This work was conducted mainly under the guidance of J. Demmel and in the first year, Marsha Berger. It involved as well A. Greenbaum, A. Mayo, Z. Bai, A. McKenney, O. Percus, J. Schmidt.

Much of the work revolved around the production of the LAPACK linear algebra library for parallel computers. This is due to be released shortly. Its goal has been to design and implement a portable linear algebra library for efficient use of high-performance supercomputers. The major methodology for making the algorithms run faster was to restructure them to perform block matrix operations in their inner loops. These functions can be optimized to exploit the memory hierarchy and gain large speed ups.

Another area has been speeding up by parallelization well known codes for linear systems arising from integral equations as well as from elliptic partial differential functions. The first produces dense and therefore more difficult linear systems - although important, too difficult to have been treated much in the past even though they are well conditioned. Work was also done analyzing a discrete-time network of queues under various circumstances. This is an important ingredient in making a parallel system work.

**Numerical Linear Algebra**

James Demmel worked on algorithms for numerical linear algebra, both from the point of view of improving their speed on supercomputers, as well as improving their accuracy. This work was done jointly with Zhaojun Bai, Anne Greenbaum and Alan McKenney. They have been part of a much larger team including researchers from U. of Tennessee and the Numercial Algorithms Group, Ltd. This is the work described above. Other results were:

"Jacobi's method is more accurate than QR" (by J. Demmel and K. Veselic, submitted to *SIAM J. Matrix Analysis and Applications* ). Shows that Jacobi's method (with a modified stopping criterion) computes small eigenvalues of symmetric positive definite matrices with uniformly higher relative accuracy than QR, divide and conquer, tradition bisection, or any algorithm which first involves tridiagonalizing the matrix. In fact, modulo an assumption based on extensive numerical tests, we show that Jacobi's method is optimally accurate in the following sense: if the matrix entries have small relative errors, so that the eigenvalues have certain intrinsic uncertainties, Jacobi will compute them with nearly this accuracy. In other words, as long as the initial matrix has small relative errors in each component, even using infinite precision will not improve on Jacobi (modulo factors of dimensionality). Does prove bisection is optimal in this sense. Also shows, the eigenvectors are computed more accurately by Jacobi (and inverse iteration) than previously thought possible. Proves similar results for using one-sided Jacobi for the singular value decomposition of a general matrix. Presents a version of Jacobi with the property that the more its accuracy exceeds that of QR, the faster it converges.

"The Bidiagonal Singular Value Decomposition and Hamiltonian Mechanics" (by P. Deift, J. Demmel, L.-C. Li, C. Tomei, accepted by *SIAM J. Numerical Analysis* ). Considers the problem of computing the singular value decomposition of a bidiagonal matrix $B$ . This problem arises in the singular value decomposition of a general matrix, and in the eigenproblem for a symmetric positive definite tridiagonal matrix. Shows that if the entries of $B$ are known with high relative accuracy, the singular values and singular vectors of $B$ will be determined to much higher accuracy than the standard perturbation theory suggest. Also shows that the algorithm in [Demmel and Kahan] computes the singular vectors as well as the singular values to this accuracy. Gives a Hamiltonian interpretation of the algorithm and use differential equation methods to prove many

of the basic facts. The Hamiltonian approach suggests a way to use flows to predict the accumulation of error in other eigenvalue algorithms as well.

"On a Block Implementation of Hessenberg Multishift QR Iteration" (by Z. Bai, J. Demmel, appeared in *International J. of High-Speed Computing*, v. 1, n. 1, 1989). The usual QR algorithm for finding the eigenvalues of a Hessenberg matrix H is based on vector-vector operations, e.g. adding a multiple of one row to another. The opportunities for parallelism in such an algorithm are limited. This paper describes a reorganizaton of the QR algorithm to permit either matrix-vector or matrix-matrix operations to be performed, both of which yield more efficient implementations on vector and parallel machines. The idea is to chase a k by k bulge rather than a 1 by 1 or 2 by 2 bulge as in the conventional QR algorithm. Preliminary numerical experiments on the CONVEX C-1 and CYBER 205 vector machines are reported.

On the Conditioning of the Nonsymmetric Eigenproblem: Theory and Software by Z. Bai, J. Demmel, A. McKenny. This report reviews the theory and practical estimation of condition numbers of the nonsymmetric eigenvalue problem. Also provides a manual for using LAPACK subroutines STRSNA and STRSEN to estimate condition numbers for individual eigenvlues and eigenvectors, multiple (or clustered) eigenvalues, and invariant subspaces.

**Iterative methods**

In addition to the work described above Anne Greenbaum has dealt with several different application areas and has focused on the use of iterative methods to solve the linear systems that rise in these different settings and on the use of parallel computing to enable more rapid solution. She has analyzed various preconditioners for the linear systems arising from self-adjoint elliptic partial differential equations and has worked on practical iterative methods for the solution of nonsymmetric linear systems. Much of the work has dealt with iterative solution of the dense linear systems that arise from integral equations. This is an area that has not received much attention from numerical linear algebraists in the past but which is sure to prove more important in the future. The matrices that arise here are dense and nonsymmetric but very well-conditioned. This means that iterative methods can be expected to converge rapidly and the major part of the

work will be in applying the matrix to a given vector at each step of the iteration. This can be done rapidly using the fast multipole method of Greengard and Rokhlin. Greenbaum worked with A. Mayo in applying these solution techniques to magnetics problems involving Laplace's or the biharmonic equation on an irregular region. She began work in applying such techniques to solve a free boundary-value problem simulating the process of Ostwald ripening. She has parallelized the adaptive version of the multipole algorithm on the NYU Ultracomputer prototype. Similar techniques are being applied to solve scattering problems described by the Helmhotz equation on an exterior region.

**Queuing Theory**

In problems of queuing arising from parallelization Ora Percus worked on

i) constructing and solving carefully chosen models in order to illuminate both local and global structure of steady state operation of clock-regulated queueing networks and on

ii) designing pseudorandom number generators for current and future parallel processors.

Switching networks in large scale digital computers are characterized by synchronous pulsed operation, and are substantially more difficult to analyze than traditional continuous time queueing systems. The control parameter in such a network is the probability $p$ of a packet entering a channel per clock cycle; in steady state, with nonsaturating queues, $p$ is constant throughout the network. The quantity of practical interest is the distribution of queue length throughout the network, since a queue which does saturate must enter another mode to allow continued operation. It is important to have a concise form for the time series transformation engendered by units of queuing networks; the combination of one mixer and two output queues, termed a $2 \times 2$ switch, is the basic unit in our initial investigation.

Since these investigations did point strongly to the fact that the near independent "light traffic" assumption was a surprisingly decent zeroth approximation up to half of the saturation flow, we continued by investigating the distribution of the queue length by an expansion of the time series in a channel about the regime of independent arrivals. Results for the second stage of such a network that we obtained recently are in very good agreement with computer simulations. This points to the possiblity that the i.i.d. input assumption that is common to virtually many

discrete queueing problems can be extended in similar fashion. In addition, the techniques we developed for obtaining the queue length distribution for the second state are expected to give us nontrivial hints as to how to work at higher stages. The work of designing pseudorandom number generators (prn's) for current and future parallel processors was pointed towards generators for MIMD (multiple instruction stream/multiple data stream) machines such as the Ultracomputer. Such architectures are very well suited for Monte Carlo calculations, since potentially independent realization or "histories" may be followed on each processor. They are much more suitable than the current generation of "vector' supercomputers for those Monte Carlo calculations with substantial logical complexity, i.e., those with data-dependent or random number determined branches. The issues addressed are applicable to many parallel machines, including existing vector-parallel machines (such as the various Crays, multipipe Cyber 205's, and the IBM 3094-400, and various hypercube machines). The emphasis has been on problems associated with very large numbers of processors.

Issues related to the design of pseudorandom number generators for MIMD parallel processors, which are particularly appropriate for Monte Carlo calculations were also analyzed to ensure reproducibility of runs, to provide very long sequences, and to assure an adequate degree of independence of the parallel streams.

## Other Topics

### The streamline diffusion finite element method

This has been examined by Anders Szepessy and is a higher order accurate implicit time stepping scheme for hyperbolic problems on general meshes. In previous work he had proved convergence of these approximations for a general scalar conservation law in several space dimensions, including also boundary conditions. It is assumed that the nonlinear discrete equations on each time step are solved exactly.

During the past year, Szepessy analysed and modified this method for systems of conservation laws.

Since the equations are nonlinear and the finite element method being considered is implicit, an iterative method has to be used to solve the discrete (nonlinear) equations at each time step. By analyzing the viscous profile, resulting from, the discretization, Szepessy proves that the above convergence result for scalar problems also holds when the nonlinear discrete equations, with $n$ degrees of freedom, are solved approximately by doing a few iterations ($<\log n$) on each time step with a simple quasi-Newton method. To obtain this, a local CFL-condition has to be satisfied. If the exact solutions of the conservation law is smooth, then the iterative method gives the same order of accuracy as solving the nonlinear discrete equations exactly.

Further, by diagonalizing and mollifying the artificial viscosity matrix in the characteristic directions, he showed that viscous profiles also exist for the approximate solutions of systems of conservation laws. This modification improves the numerical results considerably.

**Vortex Methods**

The theory of vortex methods had always been inapplicable to practical computations for two reasons: it assumed much more smoothing than is actually practical, and it relied on Eulerian derivatives of the Lagrangian variable. These derivatives grow very rapidly even for tame flows such as a vortex patch and lead to wildly pessimistic error bounds. Both of these difficulties have been eliminated in joint work with J. Goodman. First, with Cottet, Hou, and Lowengrub, convergence of the vortex method with no smoothing at all is established (the point vortex method). These convergence theorems agree with previous numerical tests and contradict a popular body of dogma. Second, with Hou, convergence theorems in weak norms that depend only on Eulerian quantities are established. Numerical experiments indeed show that errors in negative norms grow much more slowly in time than errors in strong norms. These results are contained in "Convergence of the Point Vortex Method", J. Goodman and T. Hou, to appear in Comm. Pure Appl. Math, "Convergence of a Point Vortex Method in 3D with Grid Free Stretching" G.-H. Cottet, J. Goodman and T. Hou, to appear in *SIAM J. Num. Anal.* and J. Goodman and T. Hou "New Stability Estimate for the 2-D Vortex Method" submitted to *Comm. Pure Appl. Math.*

**Viscous Shock Waves**

Together with Zhouping Xin, Goodman solved the "viscosity method problem" for piecewise smooth solutions of systems of conservation laws. They also improved the stability theory for viscous shock waves in one or two space dimensions through a number of technical improvements: the use of $L_p$ norms instead of $L_2$ and the derivation of the "integrated equations", using a "flux variable transformation rather than by integrating, and using "interaction weighted" norms to replace the complicated space-time estimates of the earlier theory. See "Viscous limits for Piecewise Smooth Solutions to Systems of Conservation Laws", in preparation and "Remarks on the Stability of Viscous Shock Profiles", preprint.

## Personnel

**Senior Personnel**

Cathleen S. Morawetz, Marsha Berger, James Demmel, Jonathan Goodman, Robert Kohn, Demetrios Christodoulou

**Research Personnel**

A. Mayo, J.P. Schmidt, J. Sylvester, Alan McKenney, Z. Bai, Anne Greenbaum, Twaidy, S. Cox, John Strain, Ora Percus, Michael Landman, Gregory Allaire, Anders Szepessy, Paula Whitlock

**Summer Research Assistants**

Yanyan Li, David Rose, Xiao Wang, Xuejan Zhang, Grotowski, Steven Cohn, Christos Michaelides, Piotr Rybka, Angie Shah, Jiangbo Lu,

**Research Assistants**

Hartosh Singh Bal, Nikan Firoozye, Carl Haverl, Marco Isopi, Tom Kreitzberg, Jordan Mann, Kevin McGrattan, Ronald Niles, David Olson, Tamara Rasmusson, Michael Tippett, Robert Young, Giovanni Zoli, Seamus O'Morain, Patrick Yen Lin, Jiangbo Lu, Christos Michaelides, Anjana Shah,

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